

# A NEW APPROXIMATION TO THE GEOMETRIC-ARITHMETIC INDEX

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**ABSTRACT.** The concept of geometric-arithmetic index was introduced in the chemical graph theory recently, but it has shown to be useful. The aim of this paper is to obtain new inequalities involving the geometric-arithmetic index  $GA_1$  and characterize graphs extremal with respect to them.

*Keywords:* Geometric-arithmetic index, Graph invariant, Vertex-degree-based graph invariant, Topological index.

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## 1. INTRODUCTION

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it in addition correlates with a molecular property it is called topological index, which is used to understand physicochemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes (see [22]).

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best known such descriptor is the Randić connectivity index ( $R$ ) [12]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (see, e.g., [5], [6], [7], [15], [16] and the references therein). During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological descriptors resembling the original Randić index. The first geometric-arithmetic index  $GA_1$ , defined in [20] as

$$GA_1 = GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$$

where  $uv$  denotes the edge of the graph  $G$  connecting the vertices  $u$  and  $v$ , and  $d_u$  is the degree of the vertex  $u$ , is one of the successors of the Randić index. Although  $GA_1$  was introduced in 2009, there are many papers dealing with this index (see, e.g., [1], [2], [3], [9], [14], [17], [20] and the references therein). There are other geometric-arithmetic indices, like  $Z_{p,q}$  ( $Z_{0,1} = GA_1$ ), but the results in [2, p.598] show that the  $GA_1$  index gathers the same information on observed molecule as other  $Z_{p,q}$  indices.

The reason for introducing a new index is to gain prediction of target property (properties) of molecules somewhat better than obtained by already presented indices. Therefore, a test study of predictive power of a new index must be done. As a standard for testing new topological descriptors, the properties of octanes are commonly used. We can find 16 physico-chemical properties of octanes at [www.molecularDescriptors.eu](http://www.molecularDescriptors.eu).

The  $GA_1$  index gives better correlation coefficients than  $R$  for these properties, but the differences between them are not significant. However, the predicting ability of the  $GA_1$  index compared with Randić index

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is reasonably better (see [2, Table 1]). Although only about 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is huge. For instance, the number of possible benzenoid hydrocarbons with 35 benzene rings is  $5.85 \cdot 10^{21}$  [19]. Therefore, the modeling of their physico-chemical properties is very important in order to predict properties of currently unknown species. The graphic in [2, Fig.7] (from [2, Table 2], [18]) shows that there exists a good linear correlation between  $GA_1$  and the heat of formation of benzenoid hydrocarbons (the correlation coefficient is equal to 0.972).

Furthermore, the improvement in prediction with  $GA_1$  index comparing to Randić index in the case of standard enthalpy of vaporization is more than 9%. That is why one can think that  $GA_1$  index should be considered in the QSPR/QSAR researches.

The aim of this paper is to obtain new inequalities involving the geometric-arithmetic index  $GA_1$  and characterize graphs extremal with respect to them.

Throughout this work,  $G = (V(G), E(G))$  denotes a (nonoriented) finite simple (without multiple edges and loops) nontrivial ( $E(G) \neq \emptyset$ ) graph.

## 2. SOME LOWER AND UPPER BOUNDS FOR $GA_1$

If  $G$  is a graph with  $m$  edges, minimum degree  $\delta$  and maximum degree  $\Delta$ , then in [1] (see also [2]) we find the bounds:

$$(2.1) \quad \frac{2m\sqrt{\delta\Delta}}{\delta + \Delta} \leq GA_1(G) \leq m.$$

Let us recall Lemma 2.2 and Corollary 2.3 in [13].

**Lemma 2.1.** *Let  $f$  be the function  $f(t) = \frac{2t}{1+t^2}$  on the interval  $[0, \infty)$ . Then  $f$  strictly increases in  $[0, 1]$ , strictly decreases in  $[1, \infty)$ ,  $f(t) = 1$  if and only if  $t = 1$  and  $f(t) = f(t_0)$  if and only if either  $t = t_0$  or  $t = t_0^{-1}$ .*

**Corollary 2.2.** *Let  $g$  be the function  $g(x, y) = \frac{2\sqrt{xy}}{x+y}$  with  $0 < a \leq x, y \leq b$ . Then*

$$\frac{2\sqrt{ab}}{a+b} \leq g(x, y) \leq 1.$$

*The equality in the lower bound is attained if and only if either  $x = a$  and  $y = b$ , or  $x = b$  and  $y = a$ , and the equality in the upper bound is attained if and only if  $x = y$ .*

The following lemma is a direct consequence of Lemma 2.1 and the fact that  $\frac{2\sqrt{xy}}{x+y} = f(t)$  with  $t = \sqrt{\frac{x}{y}}$ .

**Lemma 2.3.** *For every  $1 \leq a < b$  and every  $i \in \mathbb{N}$ ,*

$$\frac{2\sqrt{a(a+i)}}{2a+i} < \frac{2\sqrt{b(b+i)}}{2b+i}.$$

Let  $G$  be a graph with  $n$  vertices,  $m$  edges, minimum degree  $\delta$  and maximum degree  $\Delta$ . Let  $k = \Delta - \delta$  and consider the partition of the vertices given by their degrees where  $V_i$  is the set of vertices with degree  $\delta + i$  for every  $0 \leq i \leq k$ . Let  $n_i$  be the number of vertices in  $V_i$  and  $m_{ij}$  be the number of edges joining a vertex in  $V_i$  with a vertex in  $V_j$ . Then,

$$(2.2) \quad GA_1(G) = \sum_{\substack{i,j=0 \\ i \leq j}}^k \frac{2m_{ij}\sqrt{(\delta+i)(\delta+j)}}{2\delta+i+j} = \sum_{i=0}^k m_{ii} + \sum_{\substack{i,j=0 \\ i < j}}^k \frac{2m_{ij}\sqrt{(\delta+i)(\delta+j)}}{2\delta+i+j}.$$

Therefore, from this and Corollary 2.2 it is clear that  $GA_1(G) = m$  if and only if all the edges are joining vertices with equal degree. Hence,  $GA_1(G) = m$  if and only if each connected component of  $G$  is regular.

As usual, we use the convention

$$\sum_{\ell \in \emptyset} a_\ell = 0.$$

Therefore, if  $k = 0$  (i.e., if  $G$  is a regular graph), then the last sum in (2.2) is equal to zero.

Let us assume  $k = \Delta - \delta > 0$  and let  $n_i = |V_i|$  for every  $0 \leq i \leq k$ .

**Proposition 2.4.** *Let  $G$  be a nontrivial graph with minimum degree  $\delta$  and maximum degree  $\Delta > \delta$ . Then*

$$\begin{aligned} GA_1(G) &\leq \sum_{i=0}^k \min \left\{ \frac{1}{2} n_i (\delta + i), \binom{n_i}{2} \right\} + \sum_{\substack{i,j=0 \\ i < j}}^k \frac{2n_i n_j \sqrt{(\delta + i)(\delta + j)}}{2\delta + i + j} \\ &\leq \sum_{i=0}^k \min \left\{ \frac{1}{2} n_i (\delta + i), \binom{n_i}{2} \right\} + \sum_{\substack{i,j=0 \\ i < j}}^k \frac{2n_i n_j \sqrt{\Delta(\Delta - j + i)}}{2\Delta - j + i}. \end{aligned}$$

Furthermore, if  $G$  is a connected graph, then we can replace in the previous inequalities  $\frac{1}{2} n_i (\delta + i)$  by  $\frac{1}{2} n_i (\delta + i) - 1$ .

*Proof.* First, notice that in every set  $V_i$ , since there are  $n_i$  vertices,  $m_{ii} \leq \binom{n_i}{2}$ . Also, since  $d_v = \delta + i$  for every vertex  $v$  in  $V_i$ ,  $m_{ii} \leq \frac{1}{2} n_i (\delta + i)$ . Moreover, since  $V(G) \setminus V_i$  is nonempty, if  $G$  is connected, then  $m_{ii} \leq \frac{1}{2} n_i (\delta + i) - 1$ .

The number of edges joining  $V_i$  and  $V_j$  is at most  $n_i n_j$ . Thus, the result follows from (2.2) and Lemma 2.3.  $\square$

Note that the hypothesis  $\Delta > \delta$  is not essential, since if  $\Delta = \delta$  then the graph  $G$  is regular and  $GA_1(G) = m$ .

Let us consider an ordering of the vertices in  $G$  where  $u < v$  implies that  $d_u \leq d_v$ . Let us assume an orientation of the edges where  $uv$  is always considered with the orientation given by the ordering  $u < v$ . Let  $k = \Delta - \delta$ , let  $m_i$  be the number of oriented edges whose tail is a vertex with degree  $\delta + i$  and  $m'_i$  the number of oriented edges whose head is a vertex with degree  $\delta + i$  for  $0 \leq i \leq k$ . Moreover, let  $a_i$  be the number of edges whose tail is a vertex with degree  $\delta + i$  and whose head is a vertex with degree at least  $\delta + i + 1$  with  $0 \leq i \leq k - 1$ , let  $b_i$  the number of edges whose head is a vertex with degree  $\delta + i$  and whose tail is a vertex with degree at most  $\delta + i - 1$  with  $1 \leq i \leq k$ , and  $c_i$  the number of edges joining two vertices with degree  $\delta + i$  with  $0 \leq i \leq k$ . Notice that  $m_i = a_i + c_i$  and  $m'_i = b_i + c_i$  for every  $0 \leq i \leq k$ ,  $m_k = c_k$  and  $m'_0 = c_0$ .

Define the classes of graphs  $\mathcal{G}_1$ ,  $\mathcal{G}_2$  and  $\mathcal{G}_3$  as follows.  $\mathcal{G}_1$  is the set of graphs  $G$  such that if  $uv \in E(G)$ , then  $d_u = d_v$  or  $\max\{d_u, d_v\} = \Delta$ , where  $\Delta$  is the maximum degree of  $G$ .  $\mathcal{G}_2$  is the set of graphs  $G$  such that if  $uv \in E(G)$ , then  $d_u = d_v$  or  $\min\{d_u, d_v\} = \delta$ , where  $\delta$  is the minimum degree of  $G$ .  $\mathcal{G}_3$  is the set of graphs  $G$  such that if  $uv \in E(G)$ , then  $d_u = d_v$  or  $|d_u - d_v| = 1$ .

**Proposition 2.5.** *Let  $G$  be a nontrivial graph with minimum degree  $\delta$  and maximum degree  $\Delta > \delta$ . Then*

$$(2.3) \quad \sum_{i=0}^k c_i + \sum_{i=0}^{k-1} \frac{2a_i \sqrt{\Delta(\delta + i)}}{\Delta + \delta + i} \leq GA_1(G) \leq \sum_{i=0}^k c_i + \sum_{i=0}^{k-1} \frac{2a_i \sqrt{(\delta + i)(\delta + i + 1)}}{2\delta + 2i + 1},$$

and

$$(2.4) \quad \sum_{i=0}^k c_i + \sum_{i=1}^k \frac{2b_i \sqrt{\delta(\delta + i)}}{2\delta + i} \leq GA_1(G) \leq \sum_{i=0}^k c_i + \sum_{i=1}^k \frac{2b_i \sqrt{(\delta + i - 1)(\delta + i)}}{2\delta + 2i - 1}.$$

The lower bound in (2.3) is attained if and only if  $G \in \mathcal{G}_1$ . The upper bound in (2.3) is attained if and only if  $G \in \mathcal{G}_3$ . The lower bound in (2.4) is attained if and only if  $G \in \mathcal{G}_2$ . The upper bound in (2.4) is attained if and only if  $G \in \mathcal{G}_3$ .

*Proof.* Since

$$1 < \frac{\delta + i + 1}{\delta + i} \leq \frac{\delta + i + r}{\delta + i} \leq \frac{\Delta}{\delta + i}$$

for every  $1 \leq r \leq \Delta - \delta - i$  and  $f$  is decreasing on  $[1, \infty)$ , Lemma 2.1 gives

$$f\left(\sqrt{\frac{\delta+i+1}{\delta+i}}\right) \geq f\left(\sqrt{\frac{\delta+i+r}{\delta+i}}\right) \geq f\left(\sqrt{\frac{\Delta}{\delta+i}}\right).$$

Hence, (2.2) gives (2.3).

Since

$$1 < \frac{\delta+i}{\delta+i-1} \leq \frac{\delta+i}{\delta+i-r} \leq \frac{\delta+i}{\delta}$$

for every  $1 \leq r \leq i$  and  $f$  is decreasing on  $[1, \infty)$ , Lemma 2.1 gives

$$f\left(\sqrt{\frac{\delta+i}{\delta+i-1}}\right) \geq f\left(\sqrt{\frac{\delta+i}{\delta+i-r}}\right) \geq f\left(\sqrt{\frac{\delta+i}{\delta}}\right).$$

Therefore, (2.4) follows from (2.2).

One can easily check the statements on the equalities. □

**Remark 2.6.** Note that if  $C := \sum_{i=0}^k c_i$ ,  $r_i := 2a_i\sqrt{\delta+i}$  and  $r'_i := 2b_i\sqrt{\delta+i}$ , then

$$C + \sum_{i=0}^{k-1} r_i \frac{\sqrt{\Delta}}{\Delta + \delta + i} \leq GA_1(G) \leq C + \sum_{i=0}^{k-1} r_i \frac{\sqrt{\delta+i+1}}{2\delta + 2i + 1},$$

and

$$C + \sum_{i=1}^k r'_i \frac{\sqrt{\delta}}{2\delta + i} \leq GA_1(G) \leq C + \sum_{i=1}^k r'_i \frac{\sqrt{\delta+i-1}}{2\delta + 2i - 1}.$$

Define the classes of graphs  $\mathcal{G}_1^0$  and  $\mathcal{G}_2^0$  as follows.  $\mathcal{G}_1^0$  is the set of graphs  $G$  such that if  $uv \in E(G)$ , then  $\max\{d_u, d_v\} = \Delta$ , where  $\Delta$  is the maximum degree of  $G$ .  $\mathcal{G}_2^0$  is the set of graphs  $G$  such that if  $uv \in E(G)$ , then  $\min\{d_u, d_v\} = \delta$ , where  $\delta$  is the minimum degree of  $G$ . It is clear that  $\mathcal{G}_1^0 \subset \mathcal{G}_1$  and  $\mathcal{G}_2^0 \subset \mathcal{G}_2$ .

**Corollary 2.7.** Let  $G$  be a nontrivial graph with minimum degree  $\delta \geq 2$  and maximum degree  $\Delta > \delta$ . Then

$$\sum_{i=0}^k \frac{2m_i\sqrt{\Delta(\delta+i)}}{\Delta + \delta + i} = \sum_{i=0}^{k-1} \frac{2m_i\sqrt{\Delta(\delta+i)}}{\Delta + \delta + i} + m_k \leq GA_1(G) \leq m,$$

and

$$\sum_{i=0}^k \frac{2m'_i\sqrt{\delta(\delta+i)}}{2\delta + i} = m'_0 + \sum_{i=1}^k \frac{2m'_i\sqrt{\delta(\delta+i)}}{2\delta + i} \leq GA_1(G) \leq m.$$

The first (respectively, second) lower bound is attained if and only if  $G \in \mathcal{G}_1^0$  (respectively,  $G \in \mathcal{G}_2^0$ ).

Since in a connected graph with at least 3 vertices, there are no edges joining two vertices with degree 1, we have the following consequence.

**Corollary 2.8.** Let  $G$  be a nontrivial connected graph with at least 3 vertices, minimum degree 1 and maximum degree  $\Delta$ . Then

$$\sum_{i=0}^k \frac{2m_i\sqrt{\Delta(i+1)}}{\Delta + i + 1} \leq GA_1(G) \leq \frac{2\sqrt{2}m_0}{3} + \sum_{i=1}^k m_i = \frac{2\sqrt{2}m_0}{3} + m - m_0.$$

Similarly, the following result, which is Corollary 3.11 in [1], is an immediate consequence from Corollary 2.7. A vertex  $v$  is called *pendant* if the set of its neighbors has exactly one vertex, this is, if  $d_v = 1$ . Thus, with the notation above, there are  $m_0$  pendant vertices.

**Corollary 2.9.** *Let  $G$  be a nontrivial connected graph with at least 3 vertices, minimum degree 1 and minimal non-pendant vertex degree  $\delta_1$ . Then*

$$GA_1(G) \leq \frac{2m_0\sqrt{\delta_1}}{\delta_1 + 1} + m - m_0.$$

Given any graph  $G$  and  $uv \in E(G)$ , let us define the *gradient* of the edge  $uv$  as  $\nabla_{uv} := |d_u - d_v|$ .

**Proposition 2.10.** *Let  $G$  be a nontrivial graph with minimum degree  $\delta$  and maximum degree  $\Delta$ . If  $d = \min_{uv \in E(G)} \nabla_{uv}$  and  $D = \max_{uv \in E(G)} \nabla_{uv}$ , then*

$$(2.5) \quad \frac{2m\sqrt{\delta(\delta+D)}}{2\delta+D} \leq GA_1(G) \leq \frac{2m\sqrt{(\Delta-d)\Delta}}{2\Delta-d}.$$

*The equality in each inequality is attained if and only if  $G$  is either regular or bipartite with the two sets being respectively the set of vertices with degree  $\delta$  and degree  $\Delta$ .*

*Proof.* Consider any edge  $uv \in E(G)$ . By symmetry, we can assume that  $d_v \geq d_u$ . Thus,  $d \leq d_v - d_u \leq D$  and

$$\delta d_v \leq \delta d_u + \delta D \leq \delta d_u + d_u D.$$

Hence,

$$\frac{d_v}{d_u} \leq \frac{\delta + D}{\delta}$$

with equality if and only if  $d_v = d_u + D$  and  $d_u = \delta$ . Since

$$\Delta d_u \leq \Delta d_v - \Delta d \leq \Delta d_v - d_v d,$$

we have

$$\frac{\Delta}{\Delta - d} \leq \frac{d_v}{d_u}$$

with equality if and only if  $d_u = d_v - d$  and  $d_v = \Delta$ . Hence,

$$1 \leq \frac{\Delta}{\Delta - d} \leq \frac{d_v}{d_u} \leq \frac{\delta + D}{\delta},$$

and Lemma 2.1 gives

$$(2.6) \quad f\left(\sqrt{\frac{\Delta}{\Delta - d}}\right) \geq f\left(\sqrt{\frac{d_v}{d_u}}\right) \geq f\left(\sqrt{\frac{\delta + D}{\delta}}\right).$$

We obtain the inequalities in (2.5) by adding (2.6) for every  $uv \in E(G)$ .

Therefore, the equality in the lower bound is attained if and only if  $d_v = d_u + D$  and  $d_u = \delta$  for every  $uv \in E(G)$  with  $d_v \geq d_u$ ; the equality in the upper bound is attained if and only if  $d_u = d_v - d$  and  $d_v = \Delta$  for every  $uv \in E(G)$  with  $d_v \geq d_u$ . Hence, the equality in each inequality is attained if and only if  $G$  is either regular (if  $D = 0$ ) or bipartite with the two sets being respectively the set of vertices with degree  $\delta$  and degree  $\Delta$ .  $\square$

Let  $E_0, \dots, E_k$  (with  $k = \Delta - \delta$ ) be a partition of the edges of  $G$  given by the gradient where  $e \in E_i$  if  $\nabla_e = i$  for each  $0 \leq i \leq k$ . Let  $e_i$  be the number of edges in  $E_i$ .

**Proposition 2.11.** *Let  $G$  be a nontrivial graph with minimum degree  $\delta$  and maximum degree  $\Delta$ . Then*

$$(2.7) \quad \sum_{i=0}^k \frac{2e_i\sqrt{\delta(\delta+i)}}{2\delta+i} \leq GA_1(G) \leq \sum_{i=0}^k \frac{2e_i\sqrt{\Delta(\Delta-i)}}{2\Delta-i}.$$

*The upper (respectively, lower) bound is attained if and only if  $G \in \mathcal{G}_1^0$  (respectively,  $G \in \mathcal{G}_2^0$ ).*

*Proof.* Consider any edge  $uv \in E_i$ . By symmetry, we can assume that  $d_v - d_u = i$ . Since  $id_v \leq i\Delta$ , we have

$$\Delta d_u = \Delta(d_v - i) \leq \Delta d_v - id_v.$$

Hence,

$$\frac{\Delta}{\Delta - i} \leq \frac{d_v}{d_u}$$

with equality if and only if  $d_v = \Delta$ . Since  $id_v \leq id_u$ ,

$$\delta d_v = \delta(d_u + i) \leq \delta d_u + id_u,$$

and we have

$$\frac{d_v}{d_u} \leq \frac{\delta + i}{\delta}$$

with equality if and only if  $d_u = \delta$ . Therefore,

$$1 \leq \frac{\Delta}{\Delta - i} \leq \frac{d_v}{d_u} \leq \frac{\delta + i}{\delta},$$

and Lemma 2.1 gives

$$(2.8) \quad f\left(\sqrt{\frac{\Delta}{\Delta - i}}\right) \geq f\left(\sqrt{\frac{d_v}{d_u}}\right) \geq f\left(\sqrt{\frac{\delta + i}{\delta}}\right).$$

We obtain the inequalities in (2.7) by adding (2.8) for every  $uv \in E(G)$ .

Therefore, the equality in the lower bound is attained if and only if  $d_u = \delta$  for every  $uv \in E(G)$  with  $d_v \geq d_u$ ; the equality in the upper bound is attained if and only if  $d_v = \Delta$  for every  $uv \in E(G)$  with  $d_v \geq d_u$ . Hence, the upper (respectively, lower) bound is attained if and only if  $G \in \mathcal{G}_1^0$  (respectively,  $G \in \mathcal{G}_2^0$ ).  $\square$

**Remark 2.12.** *Therefore, notice that  $GA_1(G) = \frac{2m\sqrt{\delta\Delta}}{\delta+\Delta}$  if and only if  $\nabla_{uv} = \Delta - \delta$  for every edge  $uv$ . Furthermore, if  $\delta > 0$ , this occurs if and only if the graph is either regular or bipartite with the two sets being respectively the set of vertices with degree  $\delta$  and degree  $\Delta$ .*

### 3. BOUNDS INVOLVING OTHER TOPOLOGICAL INDICES

In [17, Lemma 3] appears the following result.

**Lemma 3.1.** *Let  $h$  be the function  $h(x, y) = \frac{2xy}{x+y}$  with  $\delta \leq x, y \leq \Delta$ . Then  $\delta \leq h(x, y) \leq \Delta$ . The lower (respectively, upper) bound is attained if and only if  $x = y = \delta$  (respectively,  $x = y = \Delta$ ).*

First, we obtain a lower bound of  $GA_1(G)$  depending on  $n$ ,  $m$  and  $\delta$ .

**Proposition 3.2.** *We have for any graph  $G$  with minimum degree  $\delta$ ,  $n$  vertices and  $m$  edges*

$$GA_1(G) \geq \frac{2m\sqrt{(n-1)\delta}}{n + \delta - 1},$$

*and the equality is attained if and only if  $G$  is either a complete graph or a star graph.*

*Proof.* Recall that  $\delta \leq d_u \leq n - 1$  for every  $u \in V(G)$ . By Corollary 2.2, taking  $a = \delta$  and  $b = n - 1$ , we have

$$GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \geq \sum_{uv \in E(G)} \frac{2\sqrt{(n-1)\delta}}{n + \delta - 1} = \frac{2m\sqrt{(n-1)\delta}}{n + \delta - 1}.$$

By Corollary 2.2, the equality holds for  $G$  if and only if every edge joins a vertex of degree  $\delta$  with a vertex of degree  $n - 1$ ; if  $\delta = n - 1$ , then this holds if and only if  $G$  is a complete graph; if  $\delta < n - 1$ , then this holds if and only if  $\delta = 1$  and  $G$  is a star graph.  $\square$

In what follows we will need Cassels inequality [21, Appendix 1]. Although it is a well-known result, it is not easy to find the characterization of the cases of equality. For the sake of completeness, we prove here a more general statement (following the argument of Niculescu [10]) that allows to characterize the equality.

**Lemma 3.3.** *Let  $(X, \mu)$  be a measure space and  $f, g : X \rightarrow \mathbb{R}$  non-negative measurable functions. If  $\omega f \leq g \leq \Omega f$   $\mu$ -a.e. for positive constants  $0 < \omega \leq \Omega$ , then*

$$(3.9) \quad \left( \int_X f^2 d\mu \right)^{1/2} \left( \int_X g^2 d\mu \right)^{1/2} \leq \frac{1}{2} \left( \sqrt{\frac{\Omega}{\omega}} + \sqrt{\frac{\omega}{\Omega}} \right) \int_X fg d\mu$$

and the equality is attained if and only if we have  $\omega = \Omega$  or  $f = g = 0$   $\mu$ -a.e.

*Proof.* Recall that

$$\frac{1}{\varepsilon} a^2 + \varepsilon b^2 \geq 2ab$$

and the equality holds if and only if  $a = \varepsilon b$ . Therefore, the hypotheses imply

$$\begin{aligned} 0 &\geq \int_X (g - \omega f)(g - \Omega f) d\mu = \int_X g^2 d\mu - (\Omega + \omega) \int_X fg d\mu + \Omega\omega \int_X f^2 d\mu \\ &\quad \left( \sqrt{\frac{\Omega}{\omega}} + \sqrt{\frac{\omega}{\Omega}} \right) \int_X fg d\mu \geq \frac{1}{\sqrt{\Omega\omega}} \int_X g^2 d\mu + \sqrt{\Omega\omega} \int_X f^2 d\mu \geq 2 \left( \int_X g^2 d\mu \right)^{1/2} \left( \int_X f^2 d\mu \right)^{1/2}. \end{aligned}$$

Furthermore, the equality in (3.9) holds if and only if  $(g - \omega f)(g - \Omega f) = 0$   $\mu$ -a.e. and  $\int_X g^2 d\mu = \Omega\omega \int_X f^2 d\mu$ . If  $\omega = \Omega$ , then  $g = \omega f$  and both equalities hold. Assume now that  $\omega < \Omega$ . Since  $f, g \geq 0$  and

$$\int_X g^2 d\mu = \Omega\omega \int_X f^2 d\mu \quad \Leftrightarrow \quad \int_X (g - \sqrt{\Omega\omega} f)(g + \sqrt{\Omega\omega} f) d\mu = 0,$$

the equality  $\int_X g^2 d\mu = \Omega\omega \int_X f^2 d\mu$  is equivalent to  $g = \sqrt{\Omega\omega} f$   $\mu$ -a.e. Thus,

$$0 = (g - \omega f)(g - \Omega f) = (\sqrt{\Omega\omega} - \omega)(\sqrt{\Omega\omega} - \Omega) f^2$$

and we conclude that if  $\omega < \Omega$ , then the equality in (3.9) is attained if and only if  $f = g = 0$   $\mu$ -a.e.  $\square$

We have the following direct consequence.

**Lemma 3.4.** *If  $a_j, b_j \geq 0$  and  $\omega b_j \leq a_j \leq \Omega b_j$  for  $1 \leq j \leq k$ , then*

$$\left( \sum_{j=1}^k a_j^2 \right)^{1/2} \left( \sum_{j=1}^k b_j^2 \right)^{1/2} \leq \frac{1}{2} \left( \sqrt{\frac{\Omega}{\omega}} + \sqrt{\frac{\omega}{\Omega}} \right) \sum_{j=1}^k a_j b_j.$$

If  $a_j > 0$  for some  $1 \leq j \leq k$ , then the equality holds if and only if  $\omega = \Omega$  and  $a_j = \omega b_j$  for every  $1 \leq j \leq k$ .

Recall that the *variable Zagreb index* is defined in [8] as

$$Z_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha.$$

The variable Zagreb index was used in the structure-boiling point modeling of benzenoid hydrocarbons. The obtained model is practically identical to the model based on the variable vertex-connectivity index and this is due to close relationship between the formulas for the two indices. Note that  $Z_{-1/2}$  is the usual Randić index,  $Z_1$  is the second Zagreb index  $M_2$ ,  $Z_{-1}$  is the modified Zagreb index [11], etc.

**Theorem 3.5.** *We have for any graph  $G$  with minimum degree  $\delta$ , maximum degree  $\Delta$  and  $m$  edges, and  $\alpha \in \mathbb{R}$*

$$\frac{c_{1,\alpha} m^2}{Z_\alpha(G)} \leq GA_1(G) \leq \frac{c_{2,\alpha} m^2}{Z_\alpha(G)},$$

with

$$c_{1,\alpha} := \begin{cases} \delta^{2\alpha+1} \Delta^{-1}, & \text{if } \alpha \geq -1/2, \\ \Delta^{2\alpha}, & \text{if } \alpha \leq -1/2, \end{cases} \quad c_{2,\alpha} := \begin{cases} \frac{\Delta(\Delta^{2\alpha} + \delta^{2\alpha})^2}{4\delta^{2\alpha+1}}, & \text{if } \alpha \geq -1/2, \\ \frac{(\Delta^{2\alpha} + \delta^{2\alpha})^2}{4\Delta^{2\alpha}}, & \text{if } \alpha \leq -1/2, \end{cases}$$

and each inequality is attained for some fixed  $\alpha$  if and only if  $G$  is regular.

*Proof.* Cauchy-Schwarz inequality gives

$$m^2 = \left( \sum_{uv \in E(G)} (d_u d_v)^{\alpha/2} (d_u d_v)^{-\alpha/2} \right)^2 \leq \sum_{uv \in E(G)} (d_u d_v)^\alpha \sum_{uv \in E(G)} (d_u d_v)^{-\alpha} = Z_\alpha(G) \sum_{uv \in E(G)} (d_u d_v)^{-\alpha}.$$

We have

$$GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \geq \frac{1}{\Delta} \sum_{uv \in E(G)} (d_u d_v)^{\alpha+1/2} (d_u d_v)^{-\alpha}.$$

If  $\alpha \leq -1/2$ , then

$$GA_1(G) \geq \frac{1}{\Delta} \sum_{uv \in E(G)} (d_u d_v)^{\alpha+1/2} (d_u d_v)^{-\alpha} \geq \Delta^{2\alpha} \sum_{uv \in E(G)} (d_u d_v)^{-\alpha} \geq \frac{\Delta^{2\alpha} m^2}{Z_\alpha(G)}.$$

If  $\alpha \geq -1/2$ , then

$$GA_1(G) \geq \frac{1}{\Delta} \sum_{uv \in E(G)} (d_u d_v)^{\alpha+1/2} (d_u d_v)^{-\alpha} \geq \frac{\delta^{2\alpha+1}}{\Delta} \sum_{uv \in E(G)} (d_u d_v)^{-\alpha} \geq \frac{\delta^{2\alpha+1} m^2}{\Delta Z_\alpha(G)}.$$

Hence, we obtain

$$\frac{c_{1,\alpha} m^2}{Z_\alpha(G)} \leq GA_1(G).$$

Since

$$\begin{aligned} \delta^{2\alpha} &\leq \frac{(d_u d_v)^{\alpha/2}}{(d_u d_v)^{-\alpha/2}} = (d_u d_v)^\alpha \leq \Delta^{2\alpha}, & \text{if } \alpha \geq 0, \\ \Delta^{2\alpha} &\leq \frac{(d_u d_v)^{\alpha/2}}{(d_u d_v)^{-\alpha/2}} = (d_u d_v)^\alpha \leq \delta^{2\alpha}, & \text{if } \alpha \leq 0, \end{aligned}$$

Lemma 3.4 gives

$$\begin{aligned} m^2 &= \left( \sum_{uv \in E(G)} (d_u d_v)^{\alpha/2} (d_u d_v)^{-\alpha/2} \right)^2 \geq \frac{\sum_{uv \in E(G)} (d_u d_v)^\alpha \sum_{uv \in E(G)} (d_u d_v)^{-\alpha}}{\frac{1}{4} \left( \frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha} \right)^2} \\ &= \frac{4 \Delta^{2\alpha} \delta^{2\alpha}}{(\Delta^{2\alpha} + \delta^{2\alpha})^2} Z_\alpha(G) \sum_{uv \in E(G)} (d_u d_v)^{-\alpha}. \end{aligned}$$

If  $\alpha \leq -1/2$ , then

$$\begin{aligned} GA_1(G) &\leq \frac{1}{\delta} \sum_{uv \in E(G)} (d_u d_v)^{\alpha+1/2} (d_u d_v)^{-\alpha} \leq \delta^{2\alpha} \sum_{uv \in E(G)} (d_u d_v)^{-\alpha} \\ &\leq \delta^{2\alpha} \frac{(\Delta^{2\alpha} + \delta^{2\alpha})^2}{4 \Delta^{2\alpha} \delta^{2\alpha}} \frac{m^2}{Z_\alpha(G)} = \frac{(\Delta^{2\alpha} + \delta^{2\alpha})^2}{4 \Delta^{2\alpha}} \frac{m^2}{Z_\alpha(G)}. \end{aligned}$$

If  $\alpha \geq -1/2$ , then

$$\begin{aligned} GA_1(G) &\leq \frac{1}{\delta} \sum_{uv \in E(G)} (d_u d_v)^{\alpha+1/2} (d_u d_v)^{-\alpha} \leq \frac{\Delta^{2\alpha+1}}{\delta} \sum_{uv \in E(G)} (d_u d_v)^{-\alpha} \\ &\leq \frac{\Delta^{2\alpha+1}}{\delta} \frac{(\Delta^{2\alpha} + \delta^{2\alpha})^2}{4 \Delta^{2\alpha} \delta^{2\alpha}} \frac{m^2}{Z_\alpha(G)} = \frac{\Delta(\Delta^{2\alpha} + \delta^{2\alpha})^2}{4 \delta^{2\alpha+1}} \frac{m^2}{Z_\alpha(G)}. \end{aligned}$$



Hence, we obtain

$$GA_1(G) \leq \frac{c_{2,\alpha} m^2}{Z_\alpha(G)},$$

If the graph is regular, then  $c_{1,\alpha} = c_{2,\alpha} = \Delta^{2\alpha}$ , the lower and upper bounds are the same, and they are equal to  $GA_1(G)$ . If a bound is attained for some  $\alpha$ , then we have either  $\frac{d_u+d_v}{2} = \Delta$  for every  $uv \in E(G)$  or  $\frac{d_u+d_v}{2} = \delta$  for every  $uv \in E(G)$  and we conclude that  $d_u = d_v$  for every  $u, v \in V(G)$ .  $\square$

**Corollary 3.6.** *We have for any graph  $G$  with minimum degree  $\delta$ , maximum degree  $\Delta$  and  $m$  edges*

$$\frac{\delta^3 m^2}{\Delta M_2(G)} \leq GA_1(G) \leq \frac{\Delta(\Delta^2 + \delta^2)^2 m^2}{4\delta^3 M_2(G)},$$

and each inequality is attained if and only if  $G$  is regular.

With motivation from the Randić, Zagreb and harmonic indices, the *general sum-connectivity index*  $H_\alpha$  was defined by Zhou and Trinajstić in [23] as

$$H_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha,$$

with  $\alpha \in \mathbb{R}$ . Note that  $H_1$  is the first Zagreb index  $M_1$ ,  $2H_{-1}$  is the harmonic index  $H$ ,  $H_{-1/2}$  is the sum-connectivity index, etc.

**Theorem 3.7.** *We have for any graph  $G$  with minimum degree  $\delta$  and maximum degree  $\Delta$*

$$\frac{4\Delta\delta\sqrt{M_2(G)H_{-2}(G)}}{\Delta^2 + \delta^2} \leq GA_1(G) \leq 2\sqrt{M_2(G)H_{-2}(G)}.$$

The equality in the lower bound is attained if and only if  $G$  is regular. The equality in the upper bound is attained if and only if there exists a constant  $\lambda$  such that  $d_u d_v (d_u + d_v)^2 = \lambda$  for every  $uv \in E(G)$ .

*Proof.* Cauchy-Schwarz inequality gives

$$GA_1(G)^2 = \left( \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2 \leq \sum_{uv \in E(G)} 4d_u d_v \sum_{uv \in E(G)} \frac{1}{(d_u + d_v)^2} = 4M_2(G)H_{-2}(G).$$

Since

$$4\delta^2 \leq \frac{2\sqrt{d_u d_v}}{(d_u + d_v)^{-1}} = 2\sqrt{d_u d_v} (d_u + d_v) \leq 4\Delta^2,$$

Lemma 3.4 gives

$$\begin{aligned} GA_1(G)^2 &= \left( \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2 \geq \frac{\sum_{uv \in E(G)} 4d_u d_v \sum_{uv \in E(G)} \frac{1}{(d_u + d_v)^2}}{\frac{1}{4} \left( \frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right)^2} \\ &= \frac{16\Delta^2\delta^2 M_2(G)H_{-2}(G)}{(\Delta^2 + \delta^2)^2}. \end{aligned}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to  $GA_1(G)$ .

If the lower bound is attained, then Lemma 3.4 gives that  $4\delta^2 = 4\Delta^2$  and  $G$  is regular.

If the upper bound is attained, then Cauchy-Schwarz inequality gives that

$$\frac{2\sqrt{d_u d_v}}{(d_u + d_v)^{-1}} = 2\sqrt{d_u d_v} (d_u + d_v)$$

is constant, and so there exists a constant  $\lambda$  such that  $d_u d_v (d_u + d_v)^2 = \lambda$  for every  $uv \in E(G)$ .  $\square$

We say that a graph is  $(\alpha, \beta)$ -biregular if it is a bipartite graph for which any vertex in one side of the given bipartition has degree  $\alpha$  and any vertex in the other side of the bipartition has degree  $\beta$ .

The following result characterizes in many cases the equality in the upper bound in Theorem 3.7.

**Proposition 3.8.** *Let  $G$  be a graph.*

- *If there exists a constant  $\lambda$  such that  $d_u d_v (d_u + d_v)^2 = \lambda$  for every  $uv \in E(G)$ , then each connected component of  $G$  is either regular or biregular.*
- *If  $G$  is a connected graph, then there exists a constant  $\lambda$  such that  $d_u d_v (d_u + d_v)^2 = \lambda$  for every  $uv \in E(G)$  if and only if  $G$  is either regular or biregular.*

*Proof.* Assume that there exists a constant  $\lambda$  such that  $d_u d_v (d_u + d_v)^2 = \lambda$  for every  $uv \in E(G)$ . Since the function  $f : [0, \infty) \times [0, \infty) \rightarrow \mathbb{R}$  defined as  $f(x, y) = xy(x + y)^2$  is strictly increasing in  $y$  for each fixed  $x$ , given any vertex  $u \in V(G)$ , every neighbor of  $u$  has the same degree. Hence, each connected component of  $G$  is either regular or biregular. Furthermore, if  $G$  is connected, then  $d_u d_v (d_u + d_v)^2 = \lambda$  for every  $uv \in E(G)$  if and only if  $G$  is regular or biregular.  $\square$

**Example 3.9.** *It may be wondered if there exist two different pairs of natural numbers  $a, b$  and  $c, d$  such that  $ab(a + b)^2 = cd(c + d)^2$ . The answer is affirmative and such pairs of numbers can be obtained as follows.*

*First let us choose two Pythagorean triples:  $\alpha_1, \beta_1, \gamma_1$  and  $\alpha_2, \beta_2, \gamma_2$  with  $\alpha_1 \beta_1 = \alpha_2 \beta_2$  (e.g., 12, 35, 37 and 20, 21, 29) and let  $a = \gamma_2 \alpha_1^2$ ,  $b = \gamma_2 \beta_1^2$ ,  $c = \gamma_1 \alpha_2^2$  and  $d = \gamma_1 \beta_2^2$ . Then, notice that*

$$\gamma_2 \alpha_1^2 \gamma_2 \beta_1^2 (\gamma_2 \alpha_1^2 + \gamma_2 \beta_1^2)^2 = \alpha_1^2 \beta_1^2 \gamma_1^4 \gamma_2^4 = \lambda,$$

and

$$\gamma_1 \alpha_2^2 \gamma_1 \beta_2^2 (\gamma_1 \alpha_2^2 + \gamma_1 \beta_2^2)^2 = \alpha_2^2 \beta_2^2 \gamma_1^4 \gamma_2^4 = \alpha_1^2 \beta_1^2 \gamma_1^4 \gamma_2^4 = \lambda.$$

Therefore, the best characterization of the upper bound in Theorem 3.7 is the one in Proposition 3.8.

In [17, Theorem 4] appears the inequality

$$GA_1(G) \leq \sqrt{M_2(G)Z_{-1}(G)}.$$

Note that Theorem 3.7 improves this upper bound of  $GA_1(G)$  since  $4d_u d_v \leq (d_u + d_v)^2$  gives

$$4H_{-2}(G) = \sum_{uv \in E(G)} \frac{4}{(d_u + d_v)^2} \leq \sum_{uv \in E(G)} \frac{1}{d_u d_v} = Z_{-1}(G),$$

and  $2\sqrt{H_{-2}(G)} \leq \sqrt{Z_{-1}(G)}$ .

**Theorem 3.10.** *We have for any graph  $G$  with minimum degree  $\delta$ , maximum degree  $\Delta$  and  $m$  edges*

$$\frac{\delta^2 m^2}{M_2(G)} \leq GA_1(G) \leq \frac{\Delta^{1/2}(\Delta + \delta)^3 m^2}{8 \delta^{3/2} M_2(G)},$$

and each equality is attained if and only if  $G$  is regular.

*Proof.* Lemma 3.1, Cauchy-Schwarz inequality and Corollary 2.2 give

$$\begin{aligned} (\delta m)^2 &\leq \left( \sum_{uv \in E(G)} \frac{2d_u d_v}{d_u + d_v} \right)^2 \leq \sum_{uv \in E(G)} \left( \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2 \sum_{uv \in E(G)} \left( \sqrt{d_u d_v} \right)^2 \\ &\leq \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \sum_{uv \in E(G)} d_u d_v = GA_1(G) M_2(G). \end{aligned}$$

Since

$$\frac{1}{\Delta} \leq \frac{\frac{2\sqrt{d_u d_v}}{d_u + d_v}}{\sqrt{d_u d_v}} = \frac{2}{d_u + d_v} \leq \frac{1}{\delta},$$

Lemmas 3.1, 3.4 and Corollary 2.2 give

$$\begin{aligned} (\Delta m)^2 &\geq \left( \sum_{uv \in E(G)} \frac{2d_u d_v}{d_u + d_v} \right)^2 \geq \frac{\sum_{uv \in E(G)} \left( \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2 \sum_{uv \in E(G)} \left( \sqrt{d_u d_v} \right)^2}{\frac{1}{4} \left( \sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2} \\ &\geq \frac{\frac{2\sqrt{\Delta\delta}}{\Delta + \delta} \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \sum_{uv \in E(G)} d_u d_v}{\frac{1}{4} \left( \sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2} = \frac{8(\Delta\delta)^{3/2} GA_1(G) M_2(G)}{(\Delta + \delta)^3}. \end{aligned}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to  $GA_1(G)$ .

By Lemma 3.1, if a bound is attained, then we have either  $d_u = d_v = \delta$  for every  $uv \in E(G)$  or  $d_u = d_v = \Delta$  for every  $uv \in E(G)$ , and we conclude that  $d_u = d_v$  for every  $u, v \in V(G)$ .  $\square$

Note that Theorem 3.10 improves the bounds in Corollary 3.6, since

$$\frac{\delta^3}{\Delta} \leq \delta^2, \quad \frac{\Delta^{1/2}(\Delta + \delta)^3}{8\delta^{3/2}} \leq \frac{\Delta(\Delta^2 + \delta^2)^2}{4\delta^3},$$

where the second inequality follows from

$$\begin{aligned} (s-1)(2s^8 + 2s^7 + 2s^6 + s^5 + 5s^4 + 2s^3 + 2s^2 - s + 1) &\geq 0 \quad \text{for } s \geq 1, \\ 2s^9 - s^6 + 4s^5 - 3s^4 - 3s^2 + 2s - 1 &\geq 0 \quad \text{for } s \geq 1, \\ (s^2 + 1)^3 &\leq 2s(s^4 + 1)^2 \quad \text{for } s \geq 1, \\ (t+1)^3 &\leq 2\sqrt{t}(t^2 + 1)^2 \quad \text{for } t \geq 1, \\ \delta^{3/2}(\Delta + \delta)^3 &\leq 2\Delta^{1/2}(\Delta^2 + \delta^2)^2 \quad \text{taking } t = \frac{\Delta}{\delta}. \end{aligned}$$

**Theorem 3.11.** *We have for any graph  $G$  with minimum degree  $\delta$  and maximum degree  $\Delta$*

$$\frac{H(G)^2}{Z_{-1}(G)} \leq GA_1(G) \leq \frac{(\Delta + \delta)^3 H(G)^2}{8(\Delta\delta)^{3/2} Z_{-1}(G)},$$

*and each inequality is attained if and only if  $G$  is regular.*

*Proof.* Cauchy-Schwarz inequality and Corollary 2.2 give

$$\begin{aligned} H(G)^2 &= \left( \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \right)^2 \leq \sum_{uv \in E(G)} \left( \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2 \sum_{uv \in E(G)} \left( \frac{1}{\sqrt{d_u d_v}} \right)^2 \\ &\leq \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \sum_{uv \in E(G)} \frac{1}{d_u d_v} = GA_1(G) Z_{-1}(G). \end{aligned}$$

Since Lemma 3.1 implies

$$\delta \leq \frac{\frac{2\sqrt{d_u d_v}}{d_u + d_v}}{\frac{1}{\sqrt{d_u d_v}}} = \frac{2d_u d_v}{d_u + d_v} \leq \Delta,$$

Lemma 3.4 gives

$$\begin{aligned} H(G)^2 &= \left( \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \right)^2 \geq \frac{\sum_{uv \in E(G)} \left( \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2 \sum_{uv \in E(G)} \left( \frac{1}{\sqrt{d_u d_v}} \right)^2}{\frac{1}{4} \left( \sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2} \\ &\geq \frac{\frac{2\sqrt{\Delta\delta}}{\Delta + \delta} \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \sum_{uv \in E(G)} \frac{1}{d_u d_v}}{\frac{1}{4} \left( \sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2} = \frac{8(\Delta\delta)^{3/2} GA_1(G) Z_{-1}(G)}{(\Delta + \delta)^3}. \end{aligned}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to  $GA_1(G)$ .

By Lemma 3.4, if the upper bound is attained, then  $\Delta = \delta$  and  $G$  is regular.

If the lower bound is attained, then Corollary 2.2 gives  $d_u = d_v$  for every  $uv \in E(G)$ . Cauchy-Schwarz inequality gives that there exists a constant  $\lambda$  such that

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} = \lambda \frac{1}{\sqrt{d_u d_v}}$$

for every  $uv \in E(G)$ . Hence,  $d_u = \lambda$  for every  $u \in V(G)$  and  $G$  is regular.  $\square$

The *forgotten topological index* is defined as  $F(G) = \sum_{u \in V(G)} d_u^3 = \sum_{uv \in E(G)} (d_u^2 + d_v^2)$  (see [4]).

**Theorem 3.12.** *We have for any graph  $G$  with minimum degree  $\delta$ , maximum degree  $\Delta$  and  $m$  edges*

$$2m - \frac{F(G)}{2\delta^2} \leq GA_1(G) \leq 2m - \frac{F(G)}{2\Delta^2}$$

*and each inequality is attained if and only if  $G$  is regular.*

*Proof.* The equality

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \frac{2(d_u^2 + d_v^2)}{(d_u + d_v)^2} = 2$$

and Corollary 2.2 give

$$\begin{aligned} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \frac{d_u^2 + d_v^2}{2\delta^2} &\geq 2, \\ GA_1(G) + \frac{F(G)}{2\delta^2} &\geq 2m. \end{aligned}$$

We also have

$$\begin{aligned} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \frac{d_u^2 + d_v^2}{2\Delta^2} &\leq 2, \\ GA_1(G) + \frac{F(G)}{2\Delta^2} &\leq 2m. \end{aligned}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to  $GA_1(G)$ . If a bound is attained, then we have either  $d_u + d_v = 2\delta$  for every  $uv \in E(G)$  or  $d_u^2 + d_v^2 = 2\Delta^2$  for every  $uv \in E(G)$  and we conclude that  $d_u = d_v$  for every  $u, v \in V(G)$ .  $\square$

## REFERENCES

- [1] K. C. Das, On geometric-arithmetic index of graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 619–630.
- [2] K. C. Das, I. Gutman, B. Furtula, Survey on Geometric-Arithmetic Indices of Graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 595–644.
- [3] K. C. Das, I. Gutman, B. Furtula, On first geometric-arithmetic index of graphs, *Discrete Appl. Math.* **159** (2011) 2030–2037.
- [4] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (4) (2015) 1184–1190.
- [5] I. Gutman, B. Furtula (Eds.), Recent Results in the Theory of Randić Index, Univ. Kragujevac, Kragujevac, 2008.
- [6] X. Li, I. Gutman, Mathematical Aspects of Randić Type Molecular Structure Descriptors, Univ. Kragujevac, Kragujevac, 2006.
- [7] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.
- [8] A. Miličević, S. Nikolić, On variable Zagreb indices, *Croat. Chem. Acta* **77** (2004) 97–101.
- [9] M. Mogharrab, G. H. Fath-Tabar, Some bounds on  $GA_1$  index of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2010) 33–38.
- [10] C. P. Niculescu, Converses of the Cauchy-Schwarz inequality in the  $C^*$ -framework, [https://www.researchgate.net/publication/252235293\\_Converses\\_of\\_the\\_Cauchy-Schwarz\\_inequality\\_in\\_the\\_C\\*-framework](https://www.researchgate.net/publication/252235293_Converses_of_the_Cauchy-Schwarz_inequality_in_the_C*-framework)
- [11] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb Indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
- [12] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
- [13] J. M. Rodríguez, J. M. Sigarreta, On the Geometric-Arithmetic Index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 103–120.

- [14] J. M. Rodríguez, J. M. Sigarreta, Spectral properties of geometric-arithmetic index, *Appl. Math. Comput.* **277** (2016) 142–153.
- [15] J. A. Rodríguez-Velázquez, J. M. Sigarreta, On the Randić index and conditional parameters of a graph, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 403–416.
- [16] J. A. Rodríguez-Velázquez, J. Tomás-Andreu, On the Randić index of polymeric networks modelled by generalized Sierpinski graphs, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 145–160.
- [17] J. M. Sigarreta, Bounds for the geometric-arithmetic index of a graph, *Miskolc Math. Notes* **16** (2015) 1199–1212.
- [18] TRC Thermodynamic Tables. Hydrocarbons; Thermodynamic Research Center, The Texas A & M University System: College Station, TX, 1987.
- [19] M. Vöge, A. J. Guttmann, I. Jensen, On the number of benzenoid hydrocarbons, *J. Chem. Inf. Comput. Sci.* **42** (2002) 456–466.
- [20] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.* **46** (2009) 1369–1376.
- [21] G. S. Watson, Serial correlation in regression analysis I, *Biometrika* **42** (1955) 327–342.
- [22] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
- [23] B. Zhou, N. Trinajstić, On general sum–connectivity index, *J. Math. Chem.* **47** (2010) 210–218.

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